

WRITES Program's Continued Evolution and Advancement

A. Gindhart, M. Carr, N. Ernst-Boris, A. Gasperetti, F. Rotella
International Centre for Diffraction Data
12 Campus Blvd., Newtown Square, PA USA

The drop in powder diffraction data published directly in scientific literature has continued to be significant. Many authors will mention that they did some powder diffraction analysis, but leave out the pertinent information like the reflection lists. Approximately nine years ago the International Centre for Diffraction Data (ICDD[®]) started a program called "Writes". Originally, a hard copy letter was sent to the authors of a publication of interest that mentioned powder diffraction experiments. The letter would ask the authors to provide ICDD with the data mentioned in the publication. Only a few authors would respond and generally, those few would not provide the data needed to get a full entry into the ICDD databases. This process has evolved over the past two years to sending emails, in order to get the requested information from the author faster. More responses were received, but most of the provided data were not useful for the ICDD. As an example, the data might include an experimental pattern, but no reflection list. This caused a transition in the way the Database department dealt with data that were received at the ICDD. We started to take that data and run Le Bail fits on the patterns to get a representative reflection list for the entry. This opened a whole new avenue of publishing patterns in the Powder Diffraction File[™] (PDF[®]).

More recently, we implemented an improved system for tracking the Writes data program and automated some of the author reference information required for a Writes request. Over the past year, we have had a lower return at about 8% of original requests followed by a larger return on a second request of about 17% leading to about 27% of those responses being published in the database. The hope was that by requesting quickly in the publication process, the authors would have the data more readily available, and that does appear to be the case. Lately, it seems that authors are more inclined to respond to the second request than the first. This could strictly be due to the authors putting the email aside and forgetting to send to us. One consequence however, of the improvement in author response is an increase in editorial staff data processing. More than 60% of the Writes responses are coming to us with just experimental data. This was a huge improvement over last year in which over 90% were being processed with Le Bail fits. The hope is that this continues to improve.

We still have an external editor running Le Bail fits on this data to help with the processing backlog. We believe that the increased efficiency in the process will continue to lead to an even greater response rate from authors, resulting in an increase in PDF entry publication percentage in future years for the project.

Acknowledgement: Thank you to Frank Rotella for his help in processing and running Le Bail fits on the backlog Writes data.